Butanoic acid, propyl ester

105-66-8 | DTXSID6059318

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.56 mmHg

Global applicability domain: Inside

Local applicability domain index: 9.42e-01

Confidence level: 8.92e-01

Nearest Neighbors from the Training Set

Image not found
N-Methyldiethanolamine
Measured: 5.96
Predicted: 5.88e-04

Image not found
Benzyl methyl ether
Measured: 4.80
Predicted: 1.25

Image not found
3-Octanone
Measured: 3.72
Predicted: 1.07

Image not found
Octadecamethylcyclononasiloxane
Measured: 2.59
Predicted: 3.17e-05